3-«beta»,7-«alpha»-Dihydroxy-5-androsten-17-one MO TMS

Inchi: InChI=1S/C26H47NO3Si2/c1-25-14-12-19(29-31(4,5)6)16-18(25)17-22(30-32(7,8)9)24-2

InchiKey: QQNSDFVOFMVHMI-VVLYNVHKSA-N

Formula: C26H47NO3Si2

SMILES: CON=C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 477.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	7.002		Crippen Method
rinpol	2635.00		NIST Webbook
rinpol	2635.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R386008&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices